CHE 221
Simulation Lab 6

18/03/2025

Fugacity

You are given pressure (P), compressibility factor (Z), and experimentally obtained fugacity coefficient ϕ_{exp} data and P-V data for ammonia (NH_3) at 100°C. Write MATLAB code to answer the following questions.

1. Using the P-Z-ϕ_{exp} data at 100°C calculate the fugacity coefficient ϕ_{sim} and compare its variation with the experimentally obtained fugacity coefficient (ϕ_{exp}). Is there a significant deviation? Support your answer with a suitable reason. Recall, $\Delta g = \int \frac{(Z-1)}{P}\, dP$. Read P_Z_phi.csv uisng readmatrix(). The columns in P_Z_phi.csv correspond to P (atm) in column 1, Z in column 2, and ϕ_{exp} (atm) in column 3. Use trapz() for integration. Note, the reference state is the one at the lowest P in the data.

2. Calculate Δg as a function of P using the P-V data at 100°C. Note, $\Delta g = \int v\, dP$. The columns in P_V.csv file correspond to P (atm) in column 1 and V (lit/mol) in column 2.

3. Evaluate Δg using the van der Waals equation of state data at 100°C. (use: $T_c = 405.6$ K; $P_c = 111.5$ atm) and compare the results obtained with part 2. Is there a significant deviation? Support your answer with a suitable reason. For this part you have been given a function vdw_fugacity(a,b,P,T), which returns Δg for the Van Der Walls gas. You will have to write another function that calculates the volume of the Van Der Walls gas at a given P and T and call it within vdw_fugacity(a,b,P,T). Recall, $\Delta g = RTln(\phi/\phi_0), a = \frac{27R^2T_c^2}{64P_c}$ and $b = \frac{RT_c}{8P_c}$.

4. Submit a report by Friday for all parts. Late submissions will not be accepted.